Klein paradox and antiparticle

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The Klein paradox of Klein-Gordon (KG) equation is discussed to show that KG equation is self-consistent even at one-particle level and the wave function for antiparticle is uniquely determined by the reasonable explanation of Klein paradox. No concept of "hole" is needed.

The Klein paradox of Dirac equation ([1] see also [2], [3]) is of great historical importance for cognizing the existence of antiparticle of electron (the positron) and explaining qualitatively the pair creation process in the collision of particle beam with strongly repulsive electric field. However, the explanation of this Klein paradox usually resorted to the concept of "hole" in the "negative-energy electron sea". So it was difficult to generalize to the case of Klein-Gordon (KG) equation where it is hopeless to fill the doubly infinite states of negative energy. Of course, one would say that this problem had been solved in the quantum field theory (QFT). But it is still interesting to see that it can also be understood in the category of quantum mechanics (QM).

Consider a one-dimensional problem for KG equation:

$$[i\hbar\frac{\partial}{\partial t} - V(x)]^2\psi = -c^2\hbar^2\frac{\partial^2}{\partial x^2}\psi + m^2c^4\psi \tag{1}$$

with

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & x > 0 \end{cases} \tag{2}$$

The boundary condition is fixed by incident wave function:

$$\psi_i = a\exp[\frac{i}{\hbar}(px - Et)] \qquad (x < 0) \tag{3}$$

with $p > 0$, $E = \sqrt{p^2c^2 + m^2c^4} > 0$.

We expect that the particle wave will be partially reflected at $x = 0$, forming a reflected wave ψ_r together with a transmitted wave ψ_t as follows:

$$\psi_r = b\exp[\tfrac{i}{\hbar}(-px - Et)] \qquad (x < 0) \tag{4}$$

$$\psi_t = b'\exp[\tfrac{i}{\hbar}(p'x - Et)] \qquad (x > 0) \tag{5}$$

where ${p'}^2 = (E - V_0)^2/c^2 - m^2c^2$.

The continuation condition of wave function $(\psi_i + \psi_r)$ with ψ_t at $x = 0$ leads to

$$\begin{cases} \frac{b}{a} &= \frac{p-p'}{p+p'} \\ \frac{b'}{a} &= \frac{2p}{p+p'} \end{cases} \tag{6}$$

There are two cases to be discussed:

(1)$E + mc^2 > V_0 > E$

Since $p' = \sqrt{(V_0 - E)^2/c^2 - m^2c^2} = iq$ becomes purely imaginary, the transmitted wave

$$\psi_t = b'\exp[-qx - iEt/\hbar] \qquad (x > 0) \tag{7}$$

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is decreasing exponentially along x axis while the reflectivity of incident wave equals to 1:

$$R \equiv \left| \frac{b}{a} \right|^2 = \frac{|p - iq|^2}{|p + iq|^2} = 1 \tag{8}$$

(2) $V_0 > E + mc^2$

Since now $p' = \pm\sqrt{(V_0 - E)^2/c^2 - m^2c^2}$ remains real, the transmitted wave is oscillating while the reflectivity of incident wave reads

$$R = \left| \frac{b}{a} \right|^2 = \frac{|p - p'|^2}{|p + p'|^2} = \begin{cases} < 1 & \text{if } p' > 0 \\ > 1 & \text{if } p' < 0 \end{cases} \tag{9}$$

While the result of (7) with (8) is as expected, an satisfying explanation for the prediction (9) is needed. Especially, we need to know the criterion for the choice of the sign of p' and what happens when $p' < 0$?

For this purpose, we should learn from the important observation by Feshbach and Villars, who recast the KG equation, Eq. (1), into two coupled Schrödinger equations:

$$\begin{cases} (i\hbar\frac{\partial}{\partial t} - V)\varphi &= mc^2\varphi - \frac{\hbar^2}{2m}\nabla^2(\varphi + \chi) \\ (i\hbar\frac{\partial}{\partial t} - V)\chi &= -mc^2\chi + \frac{\hbar^2}{2m}\nabla^2(\chi + \varphi) \end{cases} \tag{10}$$

with

$$\begin{cases} \varphi &= \frac{1}{2}[(1 - \frac{V}{mc^2})\psi + i\frac{\hbar}{mc^2}\dot{\psi}] \\ \chi &= \frac{1}{2}[(1 + \frac{V}{mc^2})\psi - i\frac{\hbar}{mc^2}\dot{\psi}] \end{cases} \tag{11}$$

Correspondingly, the continuity equation takes the following form,

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \vec{j} = 0 \tag{12}$$

$$\rho = \frac{i\hbar}{2mc^2}(\psi^*\dot{\psi} - \psi\dot{\psi}^*) - \frac{V}{mc^2}\psi^*\psi = \varphi^*\varphi - \chi^*\chi \tag{13}$$

$$\begin{aligned} \vec{j} &= \frac{i\hbar}{2m}(\psi\nabla\psi^* - \psi^*\nabla\psi) \\ &= \frac{i\hbar}{2m}[(\varphi\nabla\varphi^* - \varphi^*\nabla\varphi) + (\chi\nabla\chi^* - \chi^*\nabla\chi) + (\varphi\nabla\chi^* - \chi^*\nabla\varphi) + (\chi\nabla\varphi^* - \varphi^*\nabla\chi)] \end{aligned} \tag{14}$$

In the example here, we find for the incident wave ($c = 1$):

$$\begin{cases} \varphi_i &= \frac{1}{2}(1 + \frac{E}{m})\psi_i \\ \chi_i &= \frac{1}{2}(1 - \frac{E}{m})\psi_i \end{cases} \qquad (x < 0) \tag{15}$$

$$\rho_i = |\varphi_i|^2 - |\chi_i|^2 = \frac{E}{m}|a|^2 > 0 \tag{16}$$

$$j_i = \frac{p}{m}|a|^2 > 0 \tag{17}$$

For the reflected wave, one has

$$\rho_r = \frac{E}{m}|b|^2 > 0 \tag{18}$$

$$j_r = -\frac{p}{m}|b|^2 < 0 \tag{19}$$

The situation for the transmitted wave is more interesting:

$$\begin{cases} \varphi_t &= \frac{1}{2}(1+\frac{(E-V_0)}{m})\psi_t \\ \chi_t &= \frac{1}{2}(1-\frac{(E-V_0)}{m})\psi_t \end{cases} \qquad (x>0) \tag{20}$$

$$\rho_t = |\varphi_t|^2 - |\chi_t|^2 = \frac{(E-V_0)}{m}|b'|^2 < 0 \tag{21}$$

$$j_t = \frac{p'}{m}|b'|^2 \tag{22}$$

It seems quite attractive that we should demand $p' < 0$ to get $j_t < 0$ in conformity with $\rho_t < 0$ and to meet the requirement of Eq. (12) so that

$$j_i + j_r = j_t \tag{23}$$

with $|j_r| > j_i$ ($|b| > |a|$, $R > 1$).

The reason is clear. For an observer located at $x > 0$, the energy of particle in the transmitted wave should be measured with respect to the local potential V_0. In other words, the particle has energy $E' = E - V_0$ locally. Hence the wave function should be redefined as:

$$\psi_t \to \tilde{\psi_t} = b' \exp[\frac{i}{\hbar}(p'x - E't)] \qquad (x>0) \tag{24}$$

However, since $E' < 0$, from the experimental point of view, the particle with negative energy behaves as an antiparticle. We should express its wave function as:

$$\tilde{\psi_t} = b' \exp[-\frac{i}{\hbar}(|p'|x - |E'|t)] \tag{25}$$

and claim that the energy and momentum of this antiparticle are $|E'| > 0$ and $|p'| > 0$ respectively. It moves to the right though $p' < 0$ and $j_t < 0$.

So the above analysis of Klein paradox reveals that the KG equation is reasonable or self-consistent even at the one-particle level. The crucial point is looking at its wave function as a coherent superposition of two parts as shown by Eq. (11):

$$\psi = \varphi + \chi \tag{26}$$

When $|\varphi| > |\chi|$, it describes a particle like Eq. (3) with the energy and momentum operators:

$$\hat{E} = i\hbar\frac{\partial}{\partial t}, \qquad \hat{\vec{p}} = -i\hbar\nabla \tag{27}$$

When $|\chi| > |\varphi|$, it describes an antiparticle like:

$$\psi_c \sim \exp[-\frac{i}{\hbar}(\vec{p_c}\cdot\vec{x} - E_c t)] \tag{28}$$

with the corresponding operators for antiparticle:

$$\hat{E_c} = -i\hbar\frac{\partial}{\partial t}, \qquad \hat{\vec{p_c}} = i\hbar\nabla \tag{29}$$

which give $E_c > 0$ and $\vec{p_c}$ for ψ_c shown at Eq. (28). In any case, no concept of "hole" is needed.

It is interesting to notice that Eqs. (28) and (29) were pointed out long ago by Schwinger [6], Konopinski, and Mahmaud [7], and even earlier (in the Green function or propagator of QFT) by Stückelberg [8] and Feynman [9] essentially.

However, if we accept the above point of view,it will have far-reaching consequence. A particle is always not pure, it always comprises two components, φ and χ. In the equation governing its motion, φ and χ are always coupled together with the symmetry under the transformation ($\vec{x} \to -\vec{x}, t \to -t$) and

$$
\begin{aligned}
\varphi(-\vec{x},-t) &\rightarrow \chi(\vec{x},t) \\
V(-\vec{x},-t) &\rightarrow -V(\vec{x},t)
\end{aligned} \tag{30}
$$

as shown at Eq. (10) as a special case.

But we wish to stress that Eq. (30) is a basic symmetry, which should be raised as a general postulate in relativistic quantum mechanics as well as in QFT [10]. It can also be served as a starting point to understand the essence of special relativity. ([11], [5])

Finally, it is interesting to add that another paradox in physics, the original version of EPR paradox [12] also raised a very acute question in quantum mechanics. Its reasonable explanation [13] leads precisely to the same conclusion as that in this paper, i.e., the necessity of existence of antiparticle with its wave function shown as Eq.(28).

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